Abstract Submitted
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How Large are Nonadiabatic Effects in Atomic and Diatomic Systems?[1] YUBO YANG, University of Illinois Urbana Champaign, ILKKA KYLANPAA, Tampere University of Technology, NORM TUBMAN, University of California, Berkeley, JARON KROGEL, Oak Ridge National Laboratory, SHARON HAMMES-SCHIFFER, DAVID CEPERLEY, University of Illinois Urbana Champaign — We have developed a fixed-node quantum Monte Carlo method to simulate atoms and molecules without the Born-Oppenheimer approximation with sub milli-Hartree accuracy [1]. For this purpose, we construct trial wave functions with nodes that depend on both the electronic and ionic positions. We report ground-state energies and the ionization energies for the first-row atoms and atomization energies for the first-row hydrides. The latter show effects of the nonadiabatic coupling between electrons and nuclei. We discuss how the method scales to larger systems. [1] Y. Yang, I. Kylänpää, N. M. Tubman, J. T. Krogel, S. Hammes-Schiffer, D. M. Ceperley, J. Chem. Phys. **143**(12), 2015.

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